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Crystal Channelling Simulation

CATCH 1.4 User's Guide

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Abstract

The Monte Carlo program CATCH (Capture And Transport of CHarged particles in a crystal) for the simulation of planar channelling in bent crystals is presented. The program tracks a charged particle through the distorted-crystal lattice with the use of continuous-potential approximation and the non-diffusion approach to the processes of scattering on electrons and nuclei. The output consists of the exit angular distributions, the energy loss spectra, and the spectra of any close-encounter process of interest. The curvature variability, face twist, and various surface imperfections of the real crystal can be taken into account.

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1 Introduction

Channelling of a beam of charged particles in a bent monocrystal, is going to become a working tool for the next generation of accelerators [1]. Therefore there is a need for a theoretical tool which describes a whole set of experimental data on channelling in the GeV range, and which also simulates the processes important for the future applications.

The output should be the distribution of exiting primary and secondary particles, the energy loss in crystal, and any other interesting quantity related to channelling. Since these processes are sensitive to the orientation, the simulation should track every particle through the crystal lattice computing the probability of any process as a function of the co-ordinates.

Historically, one of the independent discoveries of channelling, in the early sixties, was done in a Monte Carlo simulation of low-energy (\leq MeV) ions propagating in crystals [2]. The very low ranges and the thin crystals used allowed the study of binary collisions of the incident ion with the atoms of the crystal. At GeV energy , crystals of a few centimetres in length are used, therefore tracking with binary collisions would take a considerable time. Instead, an approach with continuous potential introduced by J. Lindhard [3] can be used. In this approach one considers collisions of the incoming particle with the atomic strings or planes instead of separate atoms, if the particle is sufficiently aligned with respect to the crystallographic axis or plane. The validity of doing this improves with the increase of the particle velocity [3].

Besides the motion in the potential one must take into account the scattering. This makes it necessary to use either kinetic equations [4], or computer simulation [5] to transport particles through a crystal. The general feature of the methods described in Refs. [4, 5] is the use of the diffusion approach which omits the single scattering acts. However, in Monte Carlo methods it is easy to include the single collisions with nuclei and electrons. Besides their influence on channelling, these close-encounter processes are the source of secondary particles emitted from the crystal. Moreover, such collisions with electrons provide interesting peculiarities of the energy loss spectra in aligned crystals. Here we describe the Monte Carlo program CATCH for the simulation of planar channelling, which does not use the diffusion approximation.

To simulate the nuclear collisions we use the LUND [6] routines; the CATCH program serves as a frame to provide the orientational dependence of these processes. Another useful feature of the CATCH program is the various imperfections of the crystal surface, incorporated in the simulation because of their essential role in the crystal-assisted beam extraction. Version 1.4 of CATCH allows variable curvature of the crystal, both longitudinal and transversal, in order to set, for instance, a twist of crystal faces.

2 Continuous potential

For the potential of the atomic plane we use the Molière approximation; details can be found e.g. in the review by D. Gemmel [7]. The static-lattice potential is modified to take into account the thermal vibrations of the lattice atoms; this is done by integration

over the Gaussian distribution of the atom displacement. Bending of the crystal has no effect on this potential. However, it causes a centrifugal force in the non-inertial frame related to the atomic planes. To solve the equation of motion in the potential $U(x)$ of the bent crystal, as a first approximation to the transport of a particle,

$$pv \frac{d^2x}{dz^2} = -\frac{dU(x)}{dx} - \frac{pv}{R(z)}, \quad (1)$$

(x being the transversal, z the longitudinal coordinate, pv the particle longitudinal momentum and velocity product, $R(z)$ the local radius of curvature), we use the fast form of the Verlet algorithm [8]:

$$x_{i+1} - x_i = (\theta_i + 0.5f_i\delta z)\delta z, \quad (2)$$

$$\theta_{i+1} - \theta_i = 0.5(f_{i+1} + f_i)\delta z \quad (3)$$

with θ for dx/dz , f for the ‘force’, and δz for the step. It was chosen over the other second order algorithms for non-linear equations of motion, such as Euler-Cromer’s and Beeman’s, owing to the better conservation of the transverse energy shown in the potential motion.

Figure 1 shows the simulated phase trajectories of protons on the plane (x, θ) in Si (111). Scattering was also included; as a result, there are no channelled protons near the atomic planes. With version 1.4 of CATCH one can specify in the input cards the planar geometry equivalent either to the Si(110) geometry (equidistant planes), or to the Si(111) one. It is easy to ‘build’ any other geometry by editing the program. The bending curvature and the crystal plane orientation can be arbitrary functions of spacial coordinates. Any data measured (or assumed) for the real crystal shape can be implemented in the simulation.

3 Scattering

Beam bending by a crystal is due to the trapping of some particles in the potential well $U(x)$, where they then follow the direction of the atomic planes. This simple picture is disturbed by scattering processes which could cause (as result of one or many acts) the trapped particle to come to a free state (feed out, or de channelling process), and an initially free particle to be trapped in the channelled state (feed in, or volume capture).

3.1 Scattering on electrons

Feed out is mostly due to scattering on electrons [4], because the channelled particles keep far from the nuclei. The mean energy loss in this scattering can be written as follows [9]:

$$-\frac{dE}{dz} = \frac{D}{\beta^2} \left(0.5 \ln \frac{2m_e c^2 \beta^2 \gamma^2}{I} - \beta^2 - \frac{\delta}{2} + 0.5 \rho_e(x) \ln \frac{T_{max}}{I} \right), \quad (4)$$

with $D = 4\pi N_A r_e^2 m_e c^2 z^2 \frac{Z}{A} \rho$, z for the charge of the incident particle (in units of e), ρ for the crystal density, Z and A for atomic number and weight, and the other notation being standard [9].

The second part in the brackets is due to single collisions and depends on the local density $\rho_e(x)$ (normalized on the amorphous one) of electrons. The angle of scattering in soft acts can be computed as a random Gaussian with r.m.s. value

$$\theta_{rms}^2 = \frac{m_e}{p^2} (\delta E)_{soft}, \quad (5)$$

where $(\delta E)_{soft}$ is the soft acts contribution in Eq. (4). The probability of the hard collision contributing to the second part of Eq. (4) is computed at every step. The energy transfer T in such an act is generated according to the distribution function $P(T)$:

$$P(T) = \frac{D\rho_e(x)}{2\beta^2} \frac{1}{T^2}. \quad (6)$$

The transverse momentum transfer q is equal to

$$q = \sqrt{2m_e T + (T/c)^2}. \quad (7)$$

Its projections are used to modify the angles θ_x and θ_y of the particle.

3.2 Scattering on nuclei

The multiple Coulomb scattering on nuclei is computed by the approximation Kitagawa–Ohtsuki [10]:

$$\langle \theta_{nucl,sc}^2 \rangle = \langle \theta_{sc}^2 \rangle_{amorph} \cdot \rho_n(x) \quad (8)$$

i.e. the mean angle of scattering squared is proportional to the local density of nuclei $\rho_n(x)$. The density function is Gaussian with r.m.s. value u being the amplitude thermal vibration of the atom.

The probability of nuclear collision, proportional to $\rho_n(x)$, is checked at every step. If such a collision succeeds (then the flag ISTATU is set to -1), the LUND routine responsible for the event generation may be called. This scheme may be used for the description of any close-encounter process of interest; then one should define the collision length (ADLI in the input cards) properly. In version 1.4 of CATCH the secondary particles are normally not tracked through the crystal lattice, but their exit angles can be modified due to multiple scattering in the rest part of the crystal. In principle, a full-scale tracking of secondary particles (and even *their* products) is possible via the construction of the appropriate main program (description below) with loops and trees.

4 Crystal imperfection

The complete description of the program usage follows below. Here we show how the crystal imperfection is implemented.

4.1 Variable curvature and twist

If KRADV = 0 is set in the input cards, the transverse curvature is set to 0. The longitudinal curvature is 0 for the longitudinal coordinate z between 0 and STRAIT

(length of the forthcoming straight part), and is constant equal to $1/\text{RADIUS}$ for z between STRAIT and STRAIT + DLINA (hence DLINA means the length of the bent part).

If KRADV = 1 is set in the input cards, the curvature at any point must be defined by the user in function CURVAT. The total length of the crystal is STRAIT + DLINA in any case.

If KRADVY = 0 is set in the input cards, the orientation of the crystal planes at both entry and exit faces is constant. If KRADVY = 1 is set in the input cards, these orientations are computed according to the functions TCFROY and TCENDY, for the front face and for the back face respectively. These functions must be supplied by the user.

4.2 Surface effects

In the case of beam extraction from the accelerator, extremely small impact parameters are possible, making the surface effects essential. The particle entering the crystal very close to its edge, can suffer from various additional factors:

- miscut angle (between the atomic planes and the surface),
- roughness (i.e. non flatness) of the surface,
- possible amorphous layer,
- bent surface.

Therefore one must pay particular attention to the near-surface tracking, where the particle is entering and leaving the cristal material (due to the roughness, holes and bend), both coherent and non-coherent scattering in this peculiar region, bending in short channels, and so on. The surface effects mentioned above are simulated in the current version of CATCH. The roughness is expressed by a periodical function, $a \sin(z/\lambda)$, where a is the amplitude of ‘bumps’ and λ is their periodicity. The ‘rough’ crystalline material can be superimposed by a uniform amorphous layer. The position of surfaces is computed at every step in accordance with bending with the variable curvature. To set up these imperfections, simply give non-zero values to the corresponding parameters in the input cards.

5 Usage of routines

Figure 2 shows an example of usage of the CATCH routines. The subroutine XPREP asks for a filename with a problem description, and performs some preliminary procedures. The subroutine XCATCH takes the entry values of x , θ_x , y , θ_y and E and returns the exit values. The entry/exit values of X, Y, XP, YP and ENERGY are double precision . The units in CALL...(..) are radians and metres; the energy is returned modified according to the E loss in crystal; hitting/missing the crystal is checked, the flag for that is ISTATU (returned) :

- ISTATU = 0, crystal missed,
- ISTATU = 1, or -1, crystal hit,
- ISTATU < 0, there was nuclear interaction.

In the case of interaction one may call the necessary routines to produce the secondary particles and to get their exit parameters modified for multiple scattering. The XPOST can be called to save the histograms, to fit the data, etc. Figure 3 shows an example of the input file. The input data is listed below with comments when necessary.

- title
- KGEOM, geometry type: either 110 (equidistant planes) or 111 (planes like those in the Diamond(111) lattice)
- KTRACE, trace level:
 - if ≤ 0 , no output during tracking
 - if = 1, some output at every step of tracking
 - if ≥ 2 , all current parameters are printed at every step
- KRADV, switch on/off $R = R(z)$ option; with KRADV = 1 one must supply FUNCTION CURVAT, evaluating the curvature $1/R$ for every point; with KRADV = 0 the curvature is 1/RADIUS.
- KRADVY, switch on/off face twist; with KRADVY=1 one must supply functions TCFROY and TCENDY, evaluating the orientation of the planes for any point at the crystal faces; with KRADVY = 0 that orientation is constant.
- I1, I2, initial numbers for pseudo-random generator RAN(I1,I2)
- DZ, step size, microns. Try different DZ to be sure the result is independent of the step size. A step of the order of 1 μm is suggested for 450 GeV/c protons in Si(110). The reasonable value of DZ should be scaled like \sqrt{E} (like the oscillation period in channelling)
- ENERGY, GeV
- PMASS, mass of the beam particle, (GeV)
- RADIUS, in cm, for the bent part of the crystal. When KRADV = 1 is set, the RADIUS is used to define the histogram windows only.
- DLINA, length of the bent part of the crystal (cm). The whole length of the crystal is STRAIT + DLINA. When KRADV = 0 is set, the forthcoming part of the length STRAIT is assumed to be straight. The following part of the th DLINA is assumed to be bent with R = RADIUS.
- STRAIT, length of the forthcoming straight part, (cm)

- HDL, interplanar half-spacing, for (110) or (111)L, in Å
- HDS, interplanar half-spacing for (111)S, in Å. Must be 0 for KGEO=110
- U, thermal vibration amplitude of the lattice atoms,(Å)
- DENS, crystal density, (gram/cm³)
- RDLI, radia ion length, (cm)
- ADLI, absorption length, (cm)
- ZN, charge of the nucleus
- AN, atomic weight
- X0XTL, the crystal entry-face left-edge *x*-coordinate, (cm)
- X1XTL, the crystal entry-face right-edge *x*-coordinate, (cm)
- Y0XTL, the crystal entry-face left-edge *y*-coordinate, (cm)
- Y1XTL, the crystal entry-face right-edge *y*-coordinate, (cm)
- THXTAL, crystal angle θ_x , (μ rad)
- THYTAL, crystal angle θ_y , (μ rad)
- SKINTH, amorphous skin thickness, (cm)
Some amorphous skin with uniform thickness SKINTH can be superimposed over the surface.
- ROUGH, (cm) the roughness (= non-flatness) amplitude of every surface. It is described by some periodical function, therefore you should supply in the input both its amplitude ROUGH and period ROUGPD. It is assumed that material under the rough surface is crystalline.
- ROUGPD, surface roughness period, (cm)
- SKIMOZ, (μ rad) There is the same skin, SKINTH + ROUGH, at the entry face. If you wish, you can also set some angular spread SKIMOZ of the crystal lattice in the entry-face skin (in this skin only!). The SKIMOZ means the sigma of Gaussian distribution.
- DISCUT, miscut angle, (μ rad) Note that its sign is essential; when your impact is near the left edge of the crystal, the negative sign (DISCUT<0) is preferable.

The position of all surfaces in space, as a function of θ_x and θ_y misalignment of the crystal (THXTAL and THYTAL in the input cards), as a function of bending with variable radius, as well as a function of the surface 'rough structure', is computed at every step.

All variables read from the input cards are placed into COMMON blocks, and hence you can vary them from the main program during the execution (if you wish to scan or to optimize). Every particle (both channelled and non-channelled) is tracked in the crystal (X, Y are changed) and can leak out through any surface. Near the rough surface it is even possible to leak out and be caught again many times, i.e. the particle traverses sequentially the crystal bumps and vacuum (or amorphous skin) between. Hence, for particles touching any surface one has both Coulomb multiple and coherent collisions.

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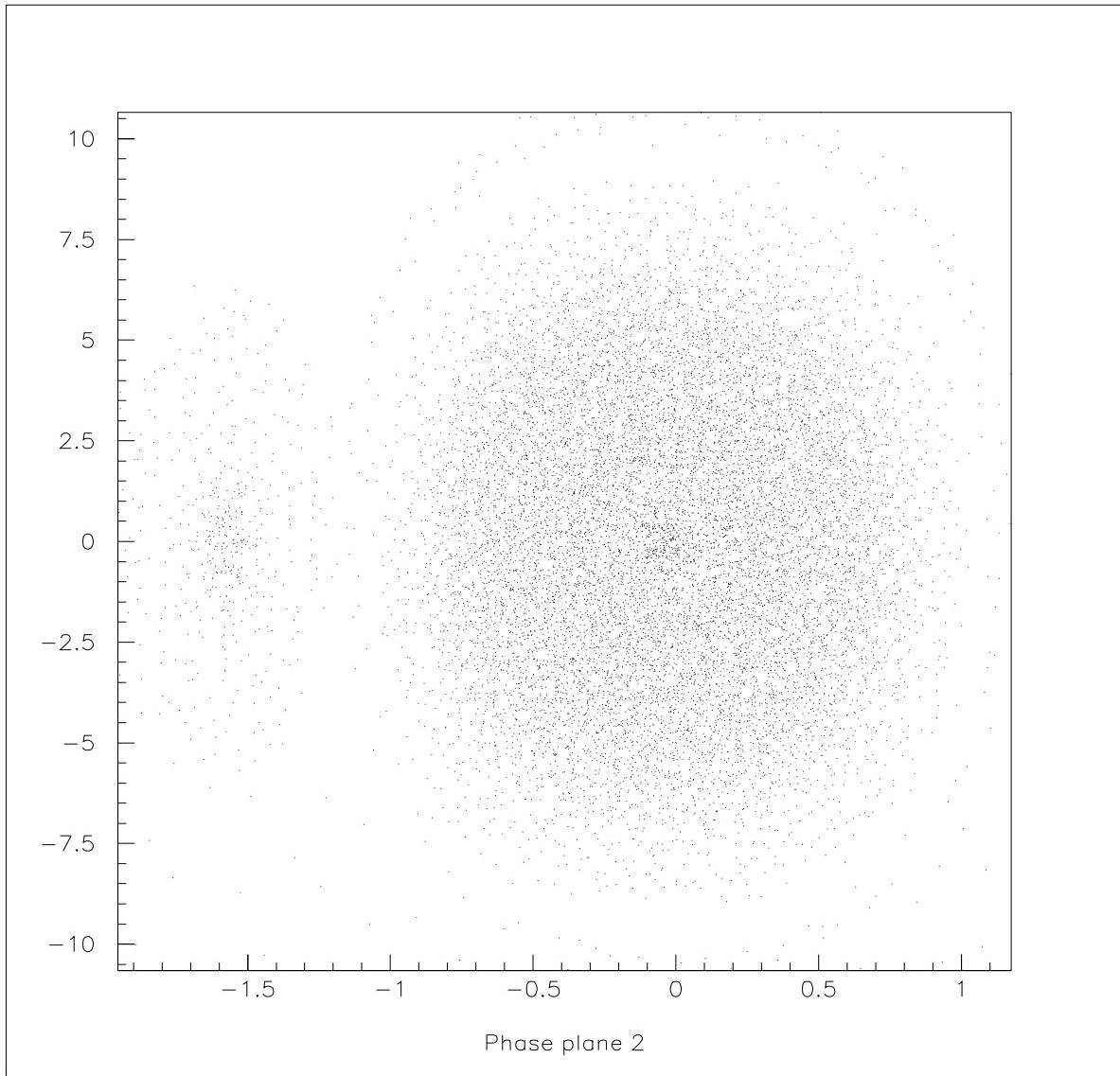


Figure 1: Phase plane angle (μ rad) vs phase plane position (\AA) of 450 GeV/c protons traced in Si(111).

```

PROGRAM XMAIN
C
C-----
C
An EXAMPLE of the
C Monte Carlo simulation
C of the planar channelling in bent crystals
C-----
DOUBLE PRECISION X,Y,XP,YP,ENERGY
C
C ...
    CALL XPREP          ! preliminary procedures
C ...
NSTAT = 100
C           statistics cycle up to NSTAT events
C ...
DO 40    IS = 1, NSTAT
C ...
XP = GAUS (0.,20.E-6)
X = 2.E-3+1.E-6*RAN(I1,I2)
YP = 0.0
Y = 0.0
ENERGY = 120.
C ...
CALL XCATCH (X,XP,Y,YP,ISTATUS,ENERGY)   ! crystal simulation
C ...
if(ISTATUS.LT.0) TYPE *, 'interacted'
C ...
TYPE *,IS, XP,YP, ISTATUS
C ...
40 CONTINUE          ! end of cycle
C ...
    CALL XPOST          ! some output
C ...
C =====
STOP
END

```

Figure 2: An example of usage of the CATCH routines

```

LHC-EXTRACTION simulation by CATCH $KEYS
  KGEOM = 110, ! geometry type
  KTRACE = 0, ! trace level
  KRADV = 0, ! switch on/off R = R(x,y,z) option
  KRADVY = 0, ! switch on/off face twist
$END
$OPTN
  I1 = 84837, ! pseudo-random start
  I2 = 53463, ! -//-
  DZ = 5., ! step size, microns
$END
$BEAM
  ENERGY = 7700., ! GeV
  PMASS = .938, ! mass of particle, GeV
$END
$CRYS
  RADIUS = 1.e4, ! cm
  DLINA = 7., ! length of bent part, cm
  STRAIT = 0., ! length of forthcoming straight part, cm
  HDL = .96, ! interplanar half-spacing, (110) or (111)L
  HDS = .0, ! interplanar half-spacing, (111)S, Angst.
  U = .075, ! thermal vibration amplitude, Angstroems
  DENS = 2.33, ! density, gramm/cm3
  RDLI = 9.38, ! radiation length, cm
  ADLI = 45., ! absorbtion length, cm
  ZN = 14., ! charge of nucleus
  AN = 28.09, ! atomic weight
$END
$GEOM
  X0XTL = 0.2, ! min X of the Xtal-face (cm)
  X1XTL = 0.5, ! max X of the Xtal-face (cm)
  Y0XTL = -.15, ! min Y of the Xtal-face (cm)
  Y1XTL = .15, ! max Y of the Xtal-face (cm)
  THXTAL = .0, ! xtal angle wrt X (microrad)
  THYTAL = .0, ! xtal angle wrt Y (microrad)
  SKINTH = 0.E-5, ! amorphous skin thickness (cm)
  ROUGH = 0.E-4, ! surface roughness (cm)
  ROUGPD = .01, ! surface roughness period (cm)
  SKIMOZ = 10., ! skin mozaicity (microrad)
  DISCUT = 0., ! miscut angle (microrad)
$END

```

Figure 3: An example of the input file